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STRUCTURE FILE UPDATES: 2 JUN 2003 HIGHEST RN 524673-75-4 DICTIONARY FILE UPDATES: 2 JUN 2003 HIGHEST RN 524673-75-4

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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(FILE 'HOME' ENTERED AT 13:11:32 ON 03 JUN 2003)

FILE 'LREGISTRY' ENTERED AT 13:12:06 ON 03 JUN 2003

L1 STR L2 STR

FILE 'REGISTRY' ENTERED AT 13:19:46 ON 03 JUN 2003

L3 SCR 1918

L4 10 S L1 AND L2 AND L3

FILE 'LREGISTRY' ENTERED AT 13:22:22 ON 03 JUN 2003 L5 STR

FILE 'REGISTRY' ENTERED AT 13:52:26 ON 03 JUN 2003

L6 1 S L1 AND L5

L7 37 S L1 AND L5 FUL SAV L7 XU409/A

FILE 'CAOLD' ENTERED AT 13:55:01 ON 03 JUN 2003 1 S L7

FILE 'ZCAPLUS' ENTERED AT 13:55:08 ON 03 JUN 2003 22 S L7

FILE 'REGISTRY' ENTERED AT 14:27:44 ON 03 JUN 2003

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VAR G1=O/S/SE/TE

VAR G2=O/S

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

L5

STR

G11 Li@3 Na@5 K@7 Zr@9 Si@11 Ti@13 Sn@15 Cs@17 Fr@19

Page 1-A

Rb @22 Hf @24 Pr @26 Pa @28 Ge @30 Pb @32 Tm @34 Md @36

Page 1-B

VAR G1=3/5/7/9/11/13/15/17/19/22/24/26/28/30/32/34/36

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L7 37 SEA FILE=REGISTRY SSS FUL L1 AND L5

100.0% PROCESSED 4752 ITERATIONS

SEARCH TIME: 00.00.01

37 ANSWERS

=> file caold FILE 'CAOLD' ENTERED AT 14:27:54 ON 03 JUN 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

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L8 ANSWER 1 OF 1 CAOLD COPYRIGHT 2003 ACS

AN CA52:20201e CAOLD

TI heterocyclic compds.

AU Moehrke, Hans; Koch, H.; Freyberg, H. v.

PA Farbwerke Hoechst Akt.-Ges.

DT Patent

PATENT NO. KIND DATE

PI DE 865305

IT 18704-67-1 63254-90-0 68287-62-7 96460-90-1 98550-00-6 98638-22-3 100546-27-8 100725-99-3 101097-57-8 **109505-71-7 109505-72-8** 109594-32-3 109601-88-9 109601-89-0 113551-28-3 116106-11-7 121968-40-9

IT 109505-71-7 109505-72-8

RN 109505-71-7 CAOLD

CN Benzenesulfonic acid, o-6-nitro-2-benzoxazolyl-, sodium salt (6CI)

(CA INDEX NAME)

Na

RN 109505-72-8 CAOLD
CN Benzenesulfonic acid, o-5-nitro-2-benzoxazolyl-, sodium salt (6CI)
(CA INDEX NAME)

Na

=> file zcaplus FILE 'ZCAPLUS' ENTERED AT 14:29:22 ON 03 JUN 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 3 Jun 2003 VOL 138 ISS 23 FILE LAST UPDATED: 2 Jun 2003 (20030602/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d l9 1-22 cbib abs hitstr hitrn

L9 ANSWER 1 OF 22 ZCAPLUS COPYRIGHT 2003 ACS

2003:200758 Document No. 138:245327 Organic electroluminescent device with boron tetraquinolinate derivative. Suzuki, Koichi; Senoo, Akihiro; Sven, Anderssen; Ueno, Kazunori (Canon Inc., Japan). Jpn. Kokai Tokkyo Koho JP 2003077671 A2 20030314, 23 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2001-265872 20010903.

AB The invention refers to an org. electroluminescent device comprising a boron tetraquinolinate deriv. (Markush structures provided) in the org. layer.

IT 501667-95-4

(org. electroluminescent device with boron tetraquinolinate deriv.)

RN 501667-95-4 ZCAPLUS

CN Borate(1-), tetrakis[2-(2-benzothiazolyl)phenolato-.kappa.O]-, lithium (9CI) (CA INDEX NAME)

PAGE 1-A

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PAGE 2-A

R2-O-S

IT 501667-95-4

(org. electroluminescent device with boron tetraquinolinate deriv.)

L9 ANSWER 2 OF 22 ZCAPLUS COPYRIGHT 2003 ACS 2003:173713 Document No. 138:228953 Organic luminescent compounds based on alkali boron complexes and organic light-emitting device using the luminescent compounds. Seok, Jai-Han (Neoview Co., Ltd., PCT Int. Appl. WO 2003018712 A1 20030306, 18 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, (English). CODEN: PIXXD2. APPLICATION: WO 2002-KR1633 20020830. PRIORITY: KR 2001-53450 20010831.

GI

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AB Org. luminescent compds. which emit light by absorbing the energy generated by electron-hole recombination are described by the general formula I, where M is Li, Na or K; X is N, O or S; and R1 to R8 are independently H, or substituted or non-substituted alkyl, aryl, heteroaryl or fused ring contain from 1 to 10 C atoms. Org. electroluminescent devices employing the org. luminescent compds. of the above formula as luminescent layer or as electron-transporting layer are also discussed.

Ι

IT 500899-12-7P

(org. luminescent compd. based on alkali boron complexes and org. light-emitting device using complexes)

RN 500899-12-7 ZCAPLUS

CN Borate(1-), tetrakis[2-(2-benzoxazolyl)-5-methylphenolato-.kappa.O]-, lithium (9CI) (CA INDEX NAME)

IT 500899-10-5P 500899-11-6P

(org. luminescent compd. based on alkali boron complexes and org. light-emitting device using complexes)

RN 500899-10-5 ZCAPLUS

CN Borate(1-), tetrakis[2-(2-benzoxazolyl)phenolato-.kappa.O]-, lithium (9CI) (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c|c}
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 & N \\
 & R - B \\
\hline
 & O - \\
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PAGE 2-A

2-0-

N O

▶ Li+

RN 500899-11-6 ZCAPLUS
CN Borate(1-), tetrakis[2-(2-benzoxazolyl)-4-methylphenolato-.kappa.0], lithium (9CI) (CA INDEX NAME)

IT 500899-12-7P

(org. luminescent compd. based on alkali boron complexes and org. light-emitting device using complexes)

IT 500899-10-5P 500899-11-6P

(org. luminescent compd. based on alkali boron complexes and org. light-emitting device using complexes)

L9 ANSWER 3 OF 22 ZCAPLUS COPYRIGHT 2003 ACS

2001:896350 Document No. 136:269793 Selective blue emission from an HPBO-Li+ complex in alkaline media. Obare, Sherine O.; Murphy, Catherine J. (Department of Chemistry and Biochemistry, Graduate Science Research Center, University of South Carolina, Columbia, SC, 29208, USA). New Journal of Chemistry, 25(12), 1600-1604 (English) 2001. CODEN: NJCHE5. ISSN: 1144-0546. Publisher: Royal Society of Chemistry.

AB 2-(2-Hydroxyphenyl)benzoxazole (HPBO) exhibits enhanced fluorescence and specificity for Li+ compared to Na+ and K+, in an alk. medium. The selectivity was obsd. in several org. solvents in the presence of bases such as pyridine, NEt3, and NMe3. HPBO-Li+ complex formation results in an intense blue emission readily obsd. by the naked eye under UV light. Spectroscopic titrns. suggest that the structure of the complex is one in which 2 HPBO anionic ligands coordinate to 1 Li+, with a 2nd Li+ as a counterion.

IT 405204-27-5

(selective blue fluorescence from an HPBO-K+ complex in alk. media)

RN 405204-27-5 ZCAPLUS

CN Phenol, 2-(2-benzoxazolyl)-, potassium salt (9CI) (CA INDEX NAME)

K

IT 259228-55-2

(selective blue fluorescence from an HPBO-Li+ complex in alk. media)

RN 259228-55-2 ZCAPLUS

CN Phenol, 2-(2-benzoxazolyl)-, lithium salt (9CI) (CA INDEX NAME)

• Li

IT 65764-88-7

(selective blue fluorescence from an HPBO-Na+ complex in alk. media)

RN 65764-88-7 ZCAPLUS

CN Phenol, 2-(2-benzoxazolyl)-, sodium salt (9CI) (CA INDEX NAME)

IT 405204-27-5

(selective blue fluorescence from an HPBO-K+ complex in alk. media)

IT 259228-55-2

(selective blue fluorescence from an HPBO-Li+ complex in alk. media)

IT 65764-88-7

(selective blue fluorescence from an HPBO-Na+ complex in alk. media)

L9 ANSWER 4 OF 22 ZCAPLUS COPYRIGHT 2003 ACS

Ι

2001:868414 Document No. 136:20006 Preparation of pyrrole derivatives as tyrosine phosphatase inhibitors for preventive and therapeutic drugs for diseases such as diabetes. Matsumoto, Takahiro; Katayama, Nozomi; Mabuchi, Hiroshi (Takeda Chemical Industries, Ltd., Japan). PCT Int. Appl. WO 2001090067 A1 20011129, 337 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (Japanese). CODEN: PIXXD2. APPLICATION: WO 2001-JP4201 20010521. PRIORITY: JP 2000-154441 20000522; JP 2000-247954 20000810.

GΙ

AB Compds. of the general formula (I) or salts thereof [wherein X1 and X2 are each a free valency or a spacer having a C1-20 main chain; one of R1 and R2 is a cyclic group which bears a substituent selected from among (1) carboxylated C1-6 alkoxy groups which may be substituted and (2) carboxylated C1-6 aliph. hydrocarbon groups which may be substituted and may further have other substituent, and the other is an optionally substituted cyclic group or hydrogen; and R3, R4 and R5 are each hydrogen or a substituent, or alternatively

R4 together with R3 or R5 may form an optionally substituted ring, with the proviso that some compds. of the general formula I are excluded.] are prepd. These compds. are useful as preventive and therapeutic drugs for diabetes, impaired glucose tolerance (IGT), tumors, autoimmune diseases, immunodeficiency, allergies, bone diseases, infections, joint diseases, hyperlipidemia, diabetes complications, obesity, cachexia, fatty liver, hypertension, liver diseases, polycystic ovary syndromes, muscular dystrophy, myocardial infarction, angina pectoris, cerebral infarction, syndrome X, high-blood insulin, inflammation, and arteriosclerosis or as improvers for insulin resistance or enhancers for insulin sensitivity or blood platelet aggregation inhibitors. cyclocondensation of 4-octylphenylamine with 1-(4-benzyloxyphenyl)-1,4-pentanedione in the presence of p-MeC6H4SO3H.H2O in PhMe under reflux for 12 h and hydrogenation of the resulting 1-(4-pentylphenyl)-2-methyl-5-(4-benzyloxyphenyl)-1H-pyrrole over 10% Pd-C in ethanol under hydrogen atm. gave 4-[1-(4-pentylphenyl)-5methyl-1H-pyrrol-2-yl]phenol which underwent Mitsunobu reaction with (S)-2-hydroxy-3-phenylpropanoic acid Et ester using 1,1'-(azocarbonyl)dipiperidine and Ph3P in PhMe at 80.degree. for 12 h to give $(2R)-2-\{[4-[1-(4-pentylphenyl)-5-methyl-1H-pyrrol-2$ yl]phenyl]oxy}-3-phenylpropanoic acid Et ester. The latter ester was converted into (2R)-2-{[4-[1-(4-pentylphenyl)-5-methyl-1H-pyrrol-2-yl]phenyl]oxy}-3-phenylpropanoic acid sodium salt (II). II showed IC50 of 0.09 .mu.M against human protein tyrosine phosphatase-1B. Tablet formulations contg. specific I, e.g. $(2R)-2-\{4-[1-[2-(4-1)]\}$ bromophenyl)ethan-1-yl]-5-methyl-1H-pyrrol-2-yl]phenoxy}-3phenylpropanoic acid, were described.

IT 376636-66-7P

(prepn. of pyrrole derivs. as tyrosine phosphatase inhibitors for preventive and therapeutic drugs for diseases such as diabetes) 376636-66-7 ZCAPLUS

RN 376636-66-7 ZCAPLUS
CN Benzenepropanoic acid, .alpha.-[4-[1-[3-[2-(2-benzoxazolyl)phenoxy]propyl]-5-methyl-1H-pyrrol-2-yl]phenoxy]-, sodium salt, (.alpha.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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 N
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 $CCH_2)_3$
 CO_2H

Na

IT 376636-66-7P

(prepn. of pyrrole derivs. as tyrosine phosphatase inhibitors for preventive and therapeutic drugs for diseases such as diabetes)

L9 ANSWER 5 OF 22 ZCAPLUS COPYRIGHT 2003 ACS

2001:851136 Document No. 136:14779 Preparation of naphthol derivatives and metal complexes. Ueno, Ryuzo; Kitayama, Masaya; Minami, Kenji; Wakamori, Hiroyuki (Kabushiki Kaisha Ueno Seiyaku Oyo Kenkyujo, Japan). PCT Int. Appl. WO 2001087859 A1 20011122, 53 pp. DESIGNATED STATES: W: CN, JP, KR, US; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR. (Japanese). CODEN: PIXXD2. APPLICATION: WO 2001-JP4006 20010515. PRIORITY: JP 2000-143219 20000516.

GΙ

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- Title compds. [I; Y1, Y2 independently = Q, ACO; A = OH, C6H5NH, O(CH2)3CH3, O(CH2)15CH3, NH(CH2)11CH3, 2-NHC6H4CH3, OCH3; X1 = O, S, NH; Z = optionally substituted arom. group or a heterocyclic group bearing a conjugated double bond; R = H, Na, alkyl, CH3CO; R1 = H, NO2], salts, various azo (mono, bis, and tris) compds., and metal complexes thereof, are prepd. as dye, org. photoreceptor, or electroluminescence material. The title compd. II was prepd. from 4,4',4''-triaminotriphenylamine and I (Y1 = Y2 = Q; X1 = S; Z = benzo; R = H; R1 = H). The title metal complex III was prepd. from title compd. I (Y1 = Y2; X1 = S; Z = benzo; R = H; R1 = H) and Cu(OAc)2.cntdot.H2O.

IT 374729-27-8P

(prepn. of naphthol derivs. and metal complexes)

RN 374729-27-8 ZCAPLUS

CN 2-Naphthalenol, 3,6-bis(2-benzothiazolyl)-, sodium salt (9CI) (CA INDEX NAME)

Na

IT 374729-27-8P

(prepn. of naphthol derivs. and metal complexes)

L9 ANSWER 6 OF 22 ZCAPLUS COPYRIGHT 2003 ACS

2001:662046 Document No. 135:359138 Preparation of mesoporous silica film containing excited-state intramolecular proton transfer (ESIPT) dye. Seo, Jangwon; Kim, Sehoon; Ogawa, Makoto; Park, Soo Young (School of Materials Science and Engineering, Seoul National University, Seoul, 151-744, S. Korea). Polymer Preprints (American Chemical Society, Division of Polymer Chemistry), 42(2), 286-287 (English) 2001. CODEN: ACPPAY. ISSN: 0032-3934. Publisher: American Chemical Society, Division of Polymer Chemistry.

AB 2-(2-Hydroxyphenyl)-6-benzoxazolecarboxylic acid 3-(triethoxysilyl)propylamide was prepd. and hydrolytically condensed with (EtO)4Si and the product was dried at 100.degree. to give a mesoporous silica film contg. a fluorescent excited-state intramol. proton transfer dye.

IT 372516-33-1P

(dye; prepn. of mesoporous silica film contg. excited-state intramol. proton transfer dye)

RN 372516-33-1 ZCAPLUS

CN 6-Benzoxazolecarboxamide, 2-(2-hydroxyphenyl)-N-[3-(triethoxysilyl)propyl]- (9CI) (CA INDEX NAME)

372516-34-2P, 2-(2-Hydroxyphenyl)-6-benzoxazolecarboxylic acid 3-(triethoxysilyl)propylamide-tetraethyl silicate copolymer (prepn. of mesoporous silica film contg. excited-state intramol. proton transfer dye)

RN 372516-34-2 ZCAPLUS

CN Silicic acid (H4SiO4), tetraethyl ester, polymer with 2-(2-hydroxyphenyl)-N-[3-(triethoxysilyl)propyl]-6-benzoxazolecarboxamide (9CI) (CA INDEX NAME)

CM 1

CRN 372516-33-1 CMF C23 H30 N2 O6 Si

$$\begin{array}{c|c} \text{OEt} & \text{O} & \text{HO} \\ \mid & \text{O} & \text{HO} \\ \mid & \text{OEt} & \text{O} \\ \mid & \text{OET} & \text{O} \end{array}$$

CM 2

CRN 78-10-4 CMF C8 H20 O4 Si

IT 372516-33-1P

(dye; prepn. of mesoporous silica film contg. excited-state intramol. proton transfer dye)

L9 ANSWER 7 OF 22 ZCAPLUS COPYRIGHT 2003 ACS

2001:621667 Document No. 135:364441 Bright pure blue emission from multilayer organic electroluminescent device with purified unidentate organometallic complex. Im, Woo-Bin; Hwang, Ha-Keun; Lee, Jae-Gyoung; Han, Kijong; Kim, Youngkyoo (NESS Center, Institute for Advanced Engineering, Kyounggi-Do, 449-860, S. Korea). Applied Physics Letters, 79(9), 1387-1389 (English) 2001. CODEN: APPLAB.

ISSN: 0003-6951. Publisher: American Institute of Physics.

Multilayer org. electroluminescent devices (OELDs) were fabricated with highly pure 2-(2-hydroxyphenyl)benzoxazolato lithium (LiPBO), which was obtained through stepwise purifn. process, as a blue emission layer. The ionization potential of the carefully purified LiPBO was .apprx.5.82 eV. The multilayer OELD with a hole-blocking layer (HBL) emitted almost pure blue light with the CIE color coordinate of x = 0.15 and y = 0.08. However, the emission color was red shifted when an electron-transporting layer (ETL) was introduced instead of the HBL. The device with both the HBL and the ETL showed stable and bright blue emission above 14,000 cd/m2 with the color coordinate of x = 0.15 and y = 0.11, even though the color purity was slightly poorer than that with only the HBL.

IT 259228-55-2

(bright pure blue emission from multilayer org. electroluminescent device comprising purified unidentate organometallic complex)

RN 259228-55-2 ZCAPLUS

CN Phenol, 2-(2-benzoxazolyl)-, lithium salt (9CI) (CA INDEX NAME)

• Li

IT 259228-55-2

(bright pure blue emission from multilayer org. electroluminescent device comprising purified unidentate organometallic complex)

L9 ANSWER 8 OF 22 ZCAPLUS COPYRIGHT 2003 ACS

2001:456078 Document No. 135:181062 End-capped carbosilane dendrimers with benzoxazole, quinoline, and pyrone derivatives. Kim, Chungkyun; Park, Eunmi (Department of Chemistry, Dong-A University, Pusan, 604-714, S. Korea). Journal of Polymer Science, Part A: Polymer Chemistry, 39(13), 2308-2314 (English) 2001. CODEN: JPACEC. ISSN: 0887-624X. Publisher: John Wiley & Sons, Inc..

Dendritic carbosilanes contg. benzoxazole, quinoline, and pyrone derivs. on the periphery were prepd. The parent dendrimers in the inner shell were prepd. by the use of iterative hydrosilylation and alkenylation cycles. The end generations were obtained by the reaction of terminal Si-Cl groups on each periphery with HOR [HOR = 2-(2-hydroxyphenyl)-benzoxazole, 8-hydroxyquinoline, and 3-hydroxy-2-methyl-4-pyrone] in the presence of amine.

IT 355833-87-3P 355833-90-8P

(prepn. and characterization of)

RN 355833-87-3 ZCAPLUS

CN Benzoxazole, 2,2',2'',2'''-[(2,4,6,8-tetramethylcyclotetrasiloxane-2,4,6,8-tetrayl)tetrakis[2,1-ethanediyl(dimethylsilylene)oxy-2,1-phenylene]]tetrakis- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 355833-90-8 ZCAPLUS

CN

PAGE 1-A

PAGE 2-B

$$-\left(\mathrm{CH_{2}}\right)_{3}-\underset{0}{\mathrm{Si-Me}}$$

PAGE 3-A

IT 355833-87-3P 355833-90-8P (prepn. and characterization of)

L9 ANSWER 9 OF 22 ZCAPLUS COPYRIGHT 2003 ACS 2000:384856 Document No. 133:144057 Non-traditional coordination in the complexes of 2-[2'-hydroxy(2'-N-tosylamino)phenyl] and 2-[(2'-hydroxyphenyl)azomethine]-1-alkylbenzimidazoles. S.; Kharisov, B. I.; Blanco, L. M.; Kuznetsova, L. I.; Garnovskii, D. A.; Volbushko, N. V.; Garnovskii, A. D. (Institute of Physical & Organic Chemistry, Rostov State University, Rostov-on-Don, 344006, Revista de la Sociedad Quimica de Mexico, 43(5), 143-148 Russia). (English) 1999. CODEN: RSQMAN. ISSN: 0583-7693. Publisher: Sociedad Quimica de Mexico.

AB The formation of mol. complexes (adducts) from benzimidazole derivs. is reported. The way of localization of the coordination bond in the synthesized compds. is also suggested. The synthesis of (LH) m.cntdot.MCln (m = 1, 2; n = 2, 4) is carried out by the interaction of typical chelating ligands 2-(hydroxy or N-tosylamino) phenylbenzazoles or 2-(2-hydroxyphenyl) azomethines of 1-alkylbenzimidazole (LH) with copper, zinc, palladium, tin and titanium chlorides (MCln). The IR, UV and luminescence studies show that nontraditional coordinations of the ligands take place in the synthesized complexes. It is suggested that the ligands exist in the complexes, probably, in the quinonoid tautomeric form, connected to the metal atom through the nitrogen atom of pyridinic type and/or oxygen atom of phenolic fragment of the ligand systems. In addn. to known std. metal chelates, the adducts with completely conserved ligand system (LH) could be also formed from the typical chelating ligands above mentioned.

IT 215670-68-1P

(prepn. of)

RN 215670-68-1 ZCAPLUS

CN Tin, bis[2-(2-benzoxazolyl-.kappa.N3)phenol]tetrachloro- (9CI) (CA INDEX NAME)

IT **215670-68-1P** (prepn. of)

L9 ANSWER 10 OF 22 ZCAPLUS COPYRIGHT 2003 ACS

2000:223923 Document No. 132:257977 Blue-emitting electroluminescent device. Takano, Akiko; Himeshima, Yoshio (Toray Industries, Inc., Japan). Jpn. Kokai Tokkyo Koho JP 2000100569 A2 20000407, 10 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1998-267853 19980922.

GI

AB A blue-emitting electroluminescent device, suited for use as a backlight in an imaging display device, comprises an alkali metal complex represented by I [x = 0, S and NR9 (R9 = H, alkyl, aryl, etc.); R1-8 = H, alkyl, cycloalkyl, etc.; M = Li, Na, K, Rb, and Sc].

Ι

IT 259228-55-2 262379-66-8

(blue-emitting electroluminescent device)

RN 259228-55-2 ZCAPLUS

CN Phenol, 2-(2-benzoxazolyl)-, lithium salt (9CI) (CA INDEX NAME)

Li

RN 262379-66-8 ZCAPLUS CN Phenol, 2-(2-benzothiazolyl)-, lithium salt (9CI) (CA INDEX NAME)

● Li

IT 259228-55-2 262379-66-8 (blue-emitting electroluminescent device)

L9 ANSWER 11 OF 22 ZCAPLUS COPYRIGHT 2003 ACS 2000:120981 Document No. 132:187445 Organometallic light-emitting substances, their manufacture, and organic electroluminescent devices using them. Kim, Young Kyu; Lee, Jae Kyung (Advanced Technical Research Institute, S. Korea). Jpn. Kokai Tokkyo Koho JP 2000053957 A2 20000222, 9 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1999-176775 19990623. PRIORITY: KR 1998-23645 19980623.

GΙ

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- The light-emitting substances comprise 8-hydroxyquinoline metal complexes I, 8-hydroxyquinolinato-5-sulfonato metal complexes II, benzoxazole or benzothiazole metal complexes III, benzotriazole metal complexes IV, or benzoquinoline metal complexes V (M1, M4 = Li, Na, K, Zr, Si, Ti, Sn, Cs, Fr, Rb, Hf, Pr, Pa, Ge, Pb, Tm, Md;

M2 = Li, Na, K, Ca, Be, Ga, Zn, Cd, Al, Cs, Fr, Rb, Be, Mg, Mn, Ti, Cu, Zr, Si, Hf, Pr, Pa, Ge, Sn, Pb, Tm, Md; M3 = Li+, Na+, K+, Cs+, Fr+, Rb+, Ca2+, Be2+, Ga3+, Zn2+, Al3+, Mg2+, Mn2+, Ti2+, Cu2+; R = H, Cl-10 alkyl; X, Y = H, Cl, F, I, Br, SO3H; A = H, F, Cl, Br, I; B = O, S, Se, Te; D = O, S; n = 1-4). 8-Hydroxyquinoline-5-sulfonato metal complexes II are manufd. by depositing or applying 8-hydroxyquinoline-5-sulfonato metal complexes I (M3 = H) and M3Z (Z = halo, OH). The electroluminescent devices have org. light-emitting layers contg. the substances. The substances show good thermal stability and give blue-, green-, or red-emitting devices with high luminescent efficiency.

IT 65764-88-7P 259228-55-2P

(organometallic light-emitting substances and their manuf. for org. electroluminescent devices)

RN 65764-88-7 ZCAPLUS

CN Phenol, 2-(2-benzoxazolyl)-, sodium salt (9CI) (CA INDEX NAME)

Na

CN

RN 259228-55-2 ZCAPLUS

Phenol, 2-(2-benzoxazolyl)-, lithium salt (9CI) (CA INDEX NAME)

● Li

IT 65764-88-7P 259228-55-2P

(organometallic light-emitting substances and their manuf. for org. electroluminescent devices)

L9 ANSWER 12 OF 22 ZCAPLUS COPYRIGHT 2003 ACS

2000:67804 Document No. 132:129805 Organic electroluminescent device.

Ueda, Hideaki; Hisamitsu, Satoshi (Minolta Camera Co., Ltd., Japan).

Jpn. Kokai Tokkyo Koho JP 2000030864 A2 20000128, 19 pp.

(Japanese). CODEN: JKXXAF. APPLICATION: JP 1998-198596 19980714.

 $\begin{bmatrix} & & \\ &$

AB An org. electroluminescent device comprises a zirconium complex represented by I [L = ligand having N and O, or N and S, coordinating atoms; and X = alkyl, alkoxy, aryl, etc.].

IT 256389-86-3 256389-91-0 (org. electroluminescent device)

RN 256389-86-3 ZCAPLUS

CN Zirconium, bis[2-(2-benzothiazolyl-.kappa.N3)phenolato-.kappa.O]oxo-(9CI) (CA INDEX NAME)

RN 256389-91-0 ZCAPLUS

CN Zirconium, bis[2-(2-benzoxazolyl-.kappa.N3)phenolato-.kappa.O]oxo-(9CI) (CA INDEX NAME)

IT 256389-86-3 256389-91-0 (org. electroluminescent device)

L9 ANSWER 13 OF 22 ZCAPLUS COPYRIGHT 2003 ACS
1999:375287 Document No. 131:5376 Silicon containing benz-x-azole compounds, cosmetic sunscreen agents containing them and their uses. Leduc, Madeleine; Richard, Herve; Lagrange, Alain (L'Oreal, Fr.). Eur. Pat. Appl. EP 921126 A1 19990609, 21 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO. (French). CODEN: EPXXDW. APPLICATION: EP 1998-402940 19981125. PRIORITY: FR 1997-15309 19971204.

GΙ

$$\begin{array}{c|c} & & & & \\ & &$$

AB Compns. contg. at least one title compd. Ra(A)SiO(3-a)/2 or ASiR1R2R3 [R = (un)satd. C1-30 hydrocarbyl, C1-8 halogenated hydrocarbyl, Me3SiO; a = 1-2; R1, R2, R3 = (un)branched, (un)satd. C1-8 alkyl or alkenyl; A = I, L = divalent radical joining A with a silicon-contg. chain; R4, R5 = H, (un)branched C1-10 alkyl, (un)branched C2-8 alkenyl, 2 adjacent R4 or R5 may form together a dioxyalkylidene group contg. 1-2 C atoms; Y = C, N; X = O, NR6, S when Y = C or C when Y = N; R6 = H, C1-8 alkyl; n, m = 1-2], useful in cosmetic sunscreen agents for skin and hair (no data), are claimed. The compds. are fat-sol., photostable, and absorb UV light well. In an example, a formulation for a sunscreen contg. II (prepn. given) is presented.

IT 225783-77-7P

(prepn. of silicon-contg. benzoxazole, benzimidazole, and other azole compds. as cosmetic sunscreen agents)

ΙI

RN 225783-77-7 ZCAPLUS

CN Phenol, 2-(2-benzoxazolyl)-4-methyl-6-[2-methyl-3-[1,3,3,3-tetramethyl-1-[(trimethylsilyl)oxy]disiloxanyl]propyl]- (9CI) (CFINDEX NAME)

IT 225783-77-7P

(prepn. of silicon-contg. benzoxazole, benzimidazole, and other azole compds. as cosmetic sunscreen agents)

L9 ANSWER 14 OF 22 ZCAPLUS COPYRIGHT 2003 ACS

- 1998:664744 Document No. 130:9966 Selective synthesis and absorption and luminescence spectral properties of coordination compounds derived from 2-[o-hydroxy(o-tolylsulfonylamino)phenyl]benzazoles. Burlov, A. S.; Kuznetsova, L. I.; Volbushko, N. V.; Korshunov, O. Yu.; Garnovskii, A. D. (Research Institute of Physical and Organic Chemistry, Rostov State University, Rostov-on-Don, Russia). Russian Journal of General Chemistry (Translation of Zhurnal Obshchei Khimii), 68(3), 463-468 (English) 1998. CODEN: RJGCEK. ISSN: 1070-3632. Publisher: MAIK Nauka/Interperiodica Publishing.
- AB Conditions for selective formation of unidentate complexes and chelates of 2-[o-hydroxy(or o-tolylsulfonylamino)phenyl]benzimidazol e and -benzoxazole were found through variation of the synthetic procedure, solvent, and initial metal salt. The absorption and luminescence spectral properties of the ligands and their complexes with zinc(II) chloride suggest that coordination increases the contribution of the quinoid structure of tautomeric 2-[o-hydroxy(o-tolylsulfonylamino)phenyl]benzazole system.

IT '215670-68-1P 215670-69-2P

(prepn. of)

RN 215670-68-1 ZCAPLUS

CN Tin, bis[2-(2-benzoxazolyl-.kappa.N3)phenol]tetrachloro- (9CI) (CA INDEX NAME)

RN 215670-69-2 ZCAPLUS CN Titanium, [2-(2-benzoxazolyl-.kappa.N3)phenol]tetrachloro- (9CI) (CA INDEX NAME)

IT 215670-68-1P 215670-69-2P (prepn. of)

L9 ANSWER 15 OF 22 ZCAPLUS COPYRIGHT 2003 ACS
1998:335635 Document No. 129:87844 Organic electroluminescent material
and organic electroluminescent device with it. Enokida, Toshio;
Tamano, Michiko; Onikubo, Shunichi; Okutsu, Satoshi (Toyo Ink Mfg.
Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 10140145 A2 19980526
Heisei, 17 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP
1996-292274 19961105.

GI

$$\begin{bmatrix}
R^2 & R^3 \\
R^1 & & & \\
X & N & & \\
R^8 & & & \\
R^7 & & & \\
R^6 & & & \\
\end{bmatrix}$$

The material has a formula I [X = O, S, NR9, CR10R11; R1-11 = CY1:CY2Y3, H, halo, cyano, NO2, OH, siloxy, acyl, CO2H, SO3H, (cyclo) alkyl, alkylthio, alkoxy, NH3, aryl, aryloxy, arylthio, heterocyclic; Y1-3 = H, cyano, (cyclo) alkyl, aryl, heterocyclic; Y2 and Y3 and adjacent groups of R1-8 may bond to form an O-, S-, or N-contg. ring; Z = C, N; M = divalent or tetravalent metal; n = 2-4 integer]. The device has a pair of electrodes sandwiching a light-emitting layer or a light-emitting layer-contg. org. compd. thin film layer, in which at least .gtoreq.1 the layers contain the material as an electron injecting substance. The device shows high luminescence and long life.

IT 209175-23-5 209175-24-6

(org. electroluminescent device contg. arom. compd. metal complex electron-injecting substance)

RN 209175-23-5 ZCAPLUS

CN

Silicic acid (H4SiO4), tetrakis[2-(2-benzothiazolyl)-6-(2-phenylethenyl)phenyl] ester (9CI) (CA INDEX NAME)

Ι

PAGE 1-A

PAGE 2-A

RN 209175-24-6 ZCAPLUS
CN Germanium, tetrakis[2-(2-benzothiazolyl-.kappa.N3)-6-(2-phenylethenyl)phenolato-.kappa.O]- (9CI) (CA INDEX NAME)

IT 209175-23-5 209175-24-6

(org. electroluminescent device contg. arom. compd. metal complex electron-injecting substance)

L9 ANSWER 16 OF 22 ZCAPLUS COPYRIGHT 2003 ACS
1996:69603 Document No. 124:177105 Aromatic and rigid rod
polyelectrolytes based on sulfonated poly(benzobisthiazoles). Kim,
Seungho; Cameron, Donald A.; Lee, Youngkwan; Reynolds, John R.;
Savage, Charles R. (Dep. Chem., Cent. Macromol. Sci. Eng. Univ.
Florida, Gainesville, FL, 32611, USA). Journal of Polymer Science,
Part A: Polymer Chemistry, 34(3), 481-92 (English) 1996. CODEN:

JPACEC. ISSN: 0887-624X. Publisher: Wiley.

Arom. polyelectrolytes based on sulfonated poly(benzobisthiazoles)
(PBTs) have been synthesized by a polycondensation reaction of sulfo-contg. arom. dicarboxylic acids with 2,5-diamino-1,4-benzenedithiol dihydrochloride (DABDT) in freshly prepd. polyphosphoric acid (PPA). Several sulfonated PBTs, poly[(benzo[1,2-d:4,5-d']bisthiazole-2,6-diyl)-2-sulfo-1,4-phenylene] sodium salt (p-sulfo PBT), poly[(benzo[1,2-d:4,5-d']bisthiazole-2,6-diyl)-5-sulfo-1,3-phenylene] sodium salt (m-sulfo PBT), their copolymers, and poly[(benzo[1,2-d:4,5-d']bisthiazole-2,6-diyl)-4,6-disulfo-1,3-phenylene] potassium salt (m-disulfo PBT), have been targeted and the polymers obtained characterized by 13C-NMR, FT-IR, elemental anal., thermal anal., and soln. viscosity

measurements. Structural analyses confirm the structures of p-sulfo PBT and m-disulfo PBT, but suggest that the sulfonate is cleaved from the chain during synthesis of m-sulfo PBT. M-disulfo PBT dissolves in water as well as strong acids, while p-sulfo PBT dissolves well in strong acids, certain solvent mixts. contg. strong acids, and hot DMSO. TGA indicates that these sulfonated PBTs are thermally stable to over 500.degree.C. Free-standing films of p-sulfo PBT, cast from dil. neutral DMSO solns., are transparent, tough, and orange in color. Films cast from basic DMSO are also free standing, while being opaque and yellow-green. P-sulfo PBT was incorporated as the dopant ion in polypyrrole, producing conductive films with conductivities as high as 3 S/cm and elec. anisotropies as high as 10.

IT 173931-08-3P

(model compd.; prepn. and characterization of arom., rigid rod
polyelectrolytes based on sulfo group-contg.
poly(benzobisthiazoles))

RN 173931-08-3 ZCAPLUS

CN Benzenesulfonic acid, 2,2'-benzo[1,2-d:4,5-d']bisthiazole-2,6-diylbis-, disodium salt (9CI) (CA INDEX NAME)

● 2 · Na

IT 173932-96-2P

(prepn. and characterization of arom., rigid rod polyelectrolytes based on sulfo group-contg. poly(benzobisthiazoles))

RN 173932-96-2 ZCAPLUS

CN Poly[benzo[1,2-d:4,5-d']bisthiazole-2,6-diyl(4,6-sulfo-1,3-phenylene) dipotassium salt] (9CI) (CA INDEX NAME)

●2 K

IT 173931-08-3P

(model compd.; prepn. and characterization of arom., rigid rod polyelectrolytes based on sulfo group-contg. poly(benzobisthiazoles))

IT 173932-96-2P

(prepn. and characterization of arom., rigid rod polyelectrolytes based on sulfo group-contg. poly(benzobisthiazoles))

- L9 ANSWER 17 OF 22 ZCAPLUS COPYRIGHT 2003 ACS
- 1988:482965 Document No. 109:82965 Removable guidepath for automated guidance vehicles. Paske, Richard, Jr.; Pallmer, Michael; King, William L., Jr. (Bell and Howell Co., USA). U.S. US 4707297 A 19871117, 10 pp. (English). CODEN: USXXAM. APPLICATION: US 1986-857729 19860429.
- AB Guidepath compns., capable of producing emitted radiation detectable by automated guidance vehicles, comprise an aq. dispersion of a fluorescent or phosphorescent compd. and .ltoreq.5 wt.% of a binder including a reversibly crosslinked ionomer. Guidepath compns. prepd. using 2-(2-(naphthylsulfonylamino)phenyl-4H-3,1-benzoxazin-4-one as the fluorescent compd. and Rhoplex B-1604 ionomer emulsion were applied to a variety of carpets and showed fair visual aesthetics, good durability (over 3 mo), and excellent deactivation characteristics (using a proprietary deactivation formula) on most carpets tested.
- IT 25389-26-8

(guidepath compns. contg. reversibly crosslinked ionomers and, for automated guidance vehicles)

RN 25389-26-8 ZCAPLUS

CN Benzenesulfonic acid, 3-(2-benzothiazolyl)-4-hydroxy-, monosodium salt (8CI, 9CI) (CA INDEX NAME)

Na

IT 25389-26-8

(guidepath compns. contg. reversibly crosslinked ionomers and, for automated guidance vehicles)

L9 ANSWER 18 OF 22 ZCAPLUS COPYRIGHT 2003 ACS

1978:169205 Document No. 88:169205 Deactivation of electron excitation in the 2-(o-hydroxyphenyl)benzoxazole molecule. Stryukov, M. B.; Lyubarskaya, A. E.; Knyazhanskii, M. I. (USSR). Zhurnal Prikladnoi Spektroskopii, 27(6), 1055-60 (Russian) 1977. CODEN: ZPSBAX. ISSN: 0514-7506.

GI

AB UV data for I (R = H, Me, Na) showed that in polar solvents (EtOH) I (R = H) existed in equil. with its ion pair form; in nonpolar solvents (hexane, C6H6) the anion band was not obsd. Excitation and luminescence spectra of I (R = H) were detd., and a deactivation scheme (diagram) was developed.

IT 65764-88-7

(UV of)

RN 65764-88-7 ZCAPLUS

CN Phenol, 2-(2-benzoxazolyl)-, sodium salt (9CI) (CA INDEX NAME)

Na

IT **65764-88-7** (UV of)

L9 ANSWER 19 OF 22 ZCAPLUS COPYRIGHT 2003 ACS
1975:92404 Document No. 82:92404 2-o-Hydroxyphenyl-6-Ndimethylaminobenzothiazole complexes of copper(II) and cobalt(II).

Moussa M N H: Shallaby A M: Taba F I M (Fac Sci Cair

Moussa, M. N. H.; Shallaby, A. M.; Taha, F. I. M. (Fac. Sci., Cairo Univ., Cairo, Egypt). Egyptian Journal of Chemistry, 16(6), 471-8 (English) 1973. CODEN: EGJCA3. ISSN: 0449-2285.

AB Complex formation of Co(II) and Cu(II) with 2-(o-hydroxyphenyl)-6-(dimethylamino)benzothiazole (HL) was studied by spectrophotometric and conductometric methods. The solid complexes [CuLCl(H2O)] (I), K[CuLCl(OH)], and [CuL(HQ)Cl(H2O)] (HQ = 8-quinolinol) were isolated. In I Cu is bound to the benzothiazole ligand through the phenolic O and the S atoms.

IT 55664-51-2P

(prepn. of)

RN 55664-51-2 ZCAPLUS

CN Cuprate(1-), chloro[2-[6-(dimethylamino)-2-benzothiazolyl]phenolato-0,S]hydroxy-, potassium (9CI) (CA INDEX NAME)

K+

IT **55664-51-2P** (prepn. of)

L9 ANSWER 20 OF 22 ZCAPLUS COPYRIGHT 2003 ACS

1971:420387 Document No. 75:20387 2-(2-Hydroxyphenyl)benzoxazoles and their antibacterial activity. Schellenbaum, Max; Duennenberger, Max (CIBA Ltd.). Patentschrift (Switz.) CH 497121 19701130, 9 pp. (German). CODEN: SWXXAS. APPLICATION: CH 1967-497121 19671031.

GI For diagram(s), see printed CA Issue.

AB The title compds. (I, R1 = H or Me; R2 is usually H, Cl, or Me; R3 and R4 are usually H or Cl; X1 and X2 are usually Cl, Br, or Me) were prepd. by condensation of 2-aminophenols with salicylic acids or by substitution of the 2-phenylbenzoxazoles. About 57 I were prepd. The min. inhibitory concns. of 17 I against Staphylococcus aureus were 0.1-300 ppm. Two naphth[1,2-d]oxazoles were also prepd.

IT 22091-70-9P 22091-71-0P

(prepn. of)

RN 22091-70-9 ZCAPLUS

CN 6-Benzoxazolesulfonic acid, 2-(3,5-dichloro-2-hydroxyphenyl)-, monosodium salt (8CI) (CA INDEX NAME)

Na

RN 22091-71-0 ZCAPLUS

CN Phenol, 2,4-dichloro-6-(5-chloro-2-benzoxazolyl)-, sodium salt (8CI) (CA INDEX NAME)

Na

IT 22091-70-9P 22091-71-0P (prepn. of)

L9 ANSWER 21 OF 22 ZCAPLUS COPYRIGHT 2003 ACS

1970:122923 Document No. 72:122923 Sodium 3-(2-benzothiazolyl)-4-hydroxybenzenesulfonate dyes and analogs. Freyermuth, Harlan B. (GAF Corp.). U.S. US 3491106 19700120, 3 pp. (English). CODEN: USXXAM. APPLICATION: US 1967-690791 19671215.

The title compds. are fluorescent dyes. Thus, 22.7 g 2- qC6H4OH (Q = 2-benzothiazolyl) was slowly added during 1 hr to 160 g 20% oleum at 10-15.degree. and the mixt. stirred overnight at room temp., poured onto 500 g ice and H2O, salted with 160 g NaCl, fil tered, slurried in 500 ml H2O, and adjusted to pH 6.5 with 45 ml 50% aq. NaOH at 25-30% to give 29.7 g 3,4-Q(H-O)C6H3SO3Na which showed a bluish-green fluorescence. Similarly was prepd. yellow fluorescent 3,2,1-Q(HO)C10H5SO3Na.

IT 25389-26-8P 25389-27-9P

(prepn. of)

RN 25389-26-8 ZCAPLUS

CN Benzenesulfonic acid, 3-(2-benzothiazolyl)-4-hydroxy-, monosodium salt (8CI, 9CI) (CA INDEX NAME)

Na

RN 25389-27-9 ZCAPLUS

CN 1-Naphthalenesulfonic acid, 3-(2-benzothiazolyl)-2-hydroxy-, monosodium salt (8CI) (CA INDEX NAME)

Na

IT 25389-26-8P 25389-27-9P (prepn. of)

L9 ANSWER 22 OF 22 ZCAPLUS COPYRIGHT 2003 ACS

1969:106498 Document No. 70:106498 Hydroxyphenyloxazole bactericides. Schellenbaum, Max; Duennenberger, Max (CIBA Ltd.). S. African ZA 6707127 19680416, 26 pp. (English). CODEN: SFXXAB. PRIORITY: CH 19661130.

GI For diagram(s), see printed CA Issue.

AB The title compds. (I) are useful for protecting various industrial products against gram-pos. and gram-neg. bacteria. Selected I killed Staphylococcus aureus and Escherichia coli at dilns. of

0.1-100 ppm. A mixt. of 20.7 g. 3,5-dichlorosalicylic acid (II), 12.3 g. 4,2-Me(H2N)C6H3OH and 100 g. polyphosphoric acid was stirred 3 hrs. at 195-200.degree. under N, then slowly poured into 2 l. iced water and the suspension stirred 1.5 hrs. to ppt. 28 g. I (R1 = R3 = R4 = H, R2 = Me, X1 = X2 = C1), m. 160-1.degree.. A mixt. of 20.7 g. II, 14.4 g. 4,2-Cl(H2N)C6H3OH, and 0.4 g. AlCl3 in 140 ml. 1,2-Cl2C6H4, kept at 130.degree., was mixed during 0.5 hr. with a soln. of 12 g. PCl3 in 10 ml. 1,2-Cl2C6H4, and refluxed 2 hrs. to give 22 g. I (R1 = R3 = R4 = H, R2 = X1 = X2 = C1), m.204-5.degree.. A soln. of 32.0 g. Br in 50 ml. HOAc was added during 80 min. to a warm (50-60.degree.) soln. of 21.1 g. 2-(2-hydroxyphenyl)-benzoxazole in 150 ml. HOAc, the suspension kept 2 hrs. at 60.degree., cooled and mixed with 200 ml. H2O and filtered to give 34 g. I (R1 = R2 = R3 = R4 = H, X1 = X2 = Br), m. 203-4.degree.. I (R1 = R2 = R3 = R4 = H, X1 = X2 = C1), m. 185.5-6.5.degree., (56.0 g.) was added during 40 min., with stirring, to 130 ml. ClSO3H, the clear soln. heated 2 hrs. at 105-10.degree. and then poured into ice water to ppt. 70 q. I (R1 = R2 = R4 = H, X1 = X2 = Cl, R3 = SO2Cl) (II), m. 264-6.degree. (dioxane). A soln. of 18.9 g. II in 50 ml. HCONMe2 was refluxed 3 hrs. to give 17 g. I (R1 = R2 = R4 = H, X1 = X2 = C1, R3 =SO3H.NHMe2) (III), m. 226-8.degree.. A mixt. of 4.05 g. III and 20 ml. of 2N NaOH was heated 15 min., cooled, and acidified with 2N HCl to give 2.6 g. I (R1 = R2 = R4 = H, R3 = SO3Na, X1 = X2 = Cl), m.>400.degree.. The tabulated compds. were similarly prepd. following compds. were also prepd. (m.p. given): IV, 230-1.degree.; V, 204-5.degree.; 2-(4-amino-2-hydroxyphenyl)-5-chlorobenzoxazole, 272-3.degree..

IT 22091-70-9P 22091-71-0P

(prepn. of)

RN 22091-70-9 ZCAPLUS

CN 6-Benzoxazolesulfonic acid, 2-(3,5-dichloro-2-hydroxyphenyl)-, monosodium salt (8CI) (CA INDEX NAME)

Na

RN 22091-71-0 ZCAPLUS

CN

Phenol, 2,4-dichloro-6-(5-chloro-2-benzoxazolyl)-, sodium salt (8CI)

(CA INDEX NAME)

Na

IT 22091-70-9P 22091-71-0P (prepn. of)